AMENDEMENT TO THE SPECIFICATION

Please amend the Abstract as follows:

ABSTRACT

A method for segregating compounds by ionization polarity ~~for use in polarity sensitive analysis thereof comprising the steps of~~ by: a) selecting a data base of a statistically significant group of compounds and determining the polarization~~, positive or negative,~~ at which each of said compounds is ionized; b) structurally analyzing the individual compounds to determine structural characteristics common to a majority of compounds which ionize at ~~positive~~ each polarity ~~and~~ to determine structural characteristics common structural characteristics, ~~to a majority of compounds which ionize at negative polarity,~~ as polarization determinants; c) sequentially arranging the polarization determinants in classification trees according to percentage determination of ~~one of said negative or positive~~ polarization; d) applying the polarization determinants in ~~one of said~~ classification trees in classifying a new compound for a predicted polarization of positive or negative at which said compound is ionized; e) segregating compounds classified as ionizing at positive polarity and compounds classified as ionizing at negative polarity; and f) separately analyzing the segregated compounds with the respective predicted polarities with an analysis instrument operable in different modes depending on ionization polarity.

Please amend the specification at page 3, line 16 through page 4, line 14 (paragraphs 0023-0027 of the published application, as indicated:

~~SHORT~~ BRIEF DESCRIPTION OF THE DRAWING

[0023] ~~The sole~~ FIGURE 1 is an example of a polarity classification tree with discrimination parameter branches and percentage of positive and negative polarities; and FIGURE 2 is a flow chart showing the steps of the present invention.

~~DETAILED DESCRIPTION OF THE INVENTION AND DRAWING~~

[0024] With reference to the classification tree 1 in ~~the~~ ~~f~~Figure 1, the number inside each node 2 of the tree indicates the fraction of the compounds with the indicated discrimination structure ionized at positive polarity, with "+" indicating present and "-" indicating absence.

[0025] As shown in ~~the f~~Figure, starting at the top of the tree, there are 698 starting compounds which were analyzed for polarity during ionization, 74% of which were ionized at a positive polarity. The compounds are separated into two groups 2a and 2b, depending on whether an OH group is present (+) or absent (-). The 210 compounds with an OH group present are less likely to be ionized at positive polarity (38%), while the 488 compounds without an OH group drop down the tree to the left and are much more likely to be ionized at positive polarity (90%) The two groups are then further segregated based on the best discriminating factor for the particular group. The 210 compounds with an OH group present are divided based on whether there are more than two oxygen atoms present. Compounds with more than two oxygen atoms are less likely to be ionized at positive polarity (23%). In contrast, compounds with less than two oxygen atoms present are more likely to be ionized at positive polarity. Every compound in all of the groups ends up in one of the four bottom leaves 3a-d of the tree with the percentages in the respective leaves serving as predictions

regarding how likely a compound with the particular structural set of discriminator structural elements will be ionized at positive polarity.

[0026] Because of the branched structure of the classification tree interactions between the effects of structural elements can be captured. Thus, the tree suggests that the number of oxygen atoms is a good discriminator for compounds but only if an OH group is present, otherwise as seen in the figure and the branches going down to the left, the presence or absence of CH.sub.2QCH.sub.2 groups, where Q is neither C or H, is a better discriminator of polarity (presence translates into 99% positive polarity).

[0027] In order to assess the potential performance of the method of the present invention, classification trees were built on 348 of the 698 compounds described above, and their predictive ability was evaluated with the remaining 350 compounds. Results based on this small sample indicates that the tree based method can accurately classify 87-89% of the compounds with respect to polarity for ionization. These data are however underestimates since the data used to generate the tree models were based on optimal ionization polarity and often a given compound will ionize at both polarities, especially where the prediction values lie near a selection threshold. Figure 2 sets forth the steps used in the above tree analysis.